# Additions and Corrections: "Force Field Calculations (MM3) on Glyoxal, Quinones, and Related Compounds," N. L. Allinger and Y. Fan, *J. Comput. Chem.*, **15**, 251 (1994)

All the data reported in this paper were calculated with MM3(92). MM3 calculates electronic energies for conjugated systems using a semi-empirical method by a VESCF (Variable-Electronegativity SCF) procedure. In the process of molecular structure optimization, the gradients of the VESCF energy contribution are not included in the total gradient. Thus, when the steric energy calculation converges and optimization stops, the VESCF energy still may change a little. Our newer versions of MM3(94,96) have tighter convergence criteria than MM3(92). Thus, the electronic energies of conjugated systems from MM3(94,96) may be slightly different from those by MM3(92). In the case of glyoxals and quinones, we found that the energies for some molecules change by up to about 1 kcal/mol from MM3(92) to MM3(94,96), and the changes should be noted for future reference. No parameter changes have been made and none are recommended. Rather, the results just do not fit experiment as well as they did previously. The following corrections are noted [all data are based on converged MM3(94,96) values]:

1. **Table IX.** The barrier for *trans-cis* glyoxal transformation is 5.62 kcal/mol, and the energy difference between *trans-cis* glyoxal is 4.41 kcal/mol. The barrier for *trans-cis* dimethylglyoxal transformation is 8.50 kcal/mol.
2. **Table XXIX.** The heat of formation from MM3 (94, 96) for *trans*-glyoxal is −52.21 kcal/mol, for Dimethylglyoxal is −77.66 kcal/mol, for *p*-benzoquinone is −30.77 kcal/mol, and for 9,10-anthraquinone is −21.17 kcal/mol.
3. **Table XXX.** The strainless heat of formation from MM3 (94, 96) for *trans*-glyoxal is −53.18 kcal/mol, for methyl glyoxal is −64.91 kcal/mol, for *p*-benzoquinone is −30.79 kcal/mol, and for 1,4-naphthaquinone is −26.37 kcal/mol.

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